

Highly Accurate Analytic Presentation of Solution of the Schrödinger Equation

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High-precision approximate analytic expressions for energies and wave functions are found for arbitrary physical potentials. The Schrödinger equation is cast into nonlinear Riccati equation, which is solved analytically in first iteration of the quasi-linearization method (QLM). The zeroth iteration is based on general features of the exact solution near the boundaries. The approach is illustrated on the Yukawa potential. The results enable accurate analytical estimates of effects of parameter variations on physical systems.

We find accurate analytic presentation of wave functions and energies for an arbitrary physical potential $U(r)$. We use the quasilinearization method (QLM) suggested recently for solving the Schrödinger equation after conversion to Riccati form [1, 2]. In QLM the nonlinear terms of the differential equation are approximated by a sequence of linear expressions. The QLM is iterative but not perturbative and gives stable solutions to nonlinear problems without depending on the existence of a smallness parameter.

Substitution of expression $y(r) = \frac{\chi'(r)}{\chi(r)}$ converts the radial Schrödinger equation $[-\frac{1}{2m} \frac{d^2}{dr^2} + U(r)]\chi(r) =$

$E\chi(r)$ into the nonlinear Riccati equation $y'(r) + y^2(r) = k^2(r)$, $k^2(r) = 2m[U(r) - E]$.

The corresponding QLM equation [1, 2] is $y'_{n+1}(r) + 2y_{n+1}y_n(r) = y_n^2(r) + k_n^2(r)$, where k_n^2 is obtained from $k^2(r)$ by replacing there E by energy of n -th iteration $E_n = \frac{\int_0^\infty \chi_n^*(r)H(r)\chi_n(r)dr}{\int_0^\infty \chi_n^*(r)\chi_n(r)dr}$, $\chi_n(r) = C \exp(\lambda \int^r y_n(r')dr')$. Since the QLM iterations have very fast quadratic convergence [1, 2], one can expect that even the first iteration which is given by an analytic expression [3]

$$y_1(r) = \int_0^r e^{2 \int_r^s y_0(t)dt} [y_0^2(s) + k^2(s)] ds = \frac{1}{\chi_0^2(r)} \int_0^r \chi_0^2(s) [y_0^2(s) + k_0^2(s)] ds. \quad (1)$$

will be accurate if the zeroth iteration based on general features of solutions near the boundaries is chosen.

For illustration we find the wave functions and binding energies of Yukawa potential analytically in the first QLM iteration. To estimate the precision of our analytic solution we solve the Schrödinger equation numerically as well.

The Yukawa potential $U(r) = -g \frac{e^{-\lambda r}}{r}$, $g > 0$ was suggested in the early days of quantum mechanics for description of nucleon interactions. During last decades the Yukawa potential have been used in atomic physics applications, such as the screening of nucleon electromagnetic field by electron cloud, or atoms under external pressure and in connection to quark interactions with parameters λ and g depending on the temperature of the quark-gluon plasma.

Let us try to guess the simplest form of the wave function. The large distance behavior is $\psi(r) \sim e^{-\eta r}$ with $\eta = \sqrt{-2mE}$, while the small distance behavior is determined by the Kato condition [4] $\psi(0) = -\frac{\psi'(0)}{\mu}$ with $\mu = mg$. Noting also that the radial wave function should have a nonzero value at the origin, we come to the following initial guess function $\psi_0(r) \sim \frac{e^{-\eta r} - e^{-a r}}{r}$ with a chosen to satisfy the Kato condition which leads to $a = 2\mu - \eta$. Thus we find for the initial guess $\chi_0(r) = r\psi_0(r) = N [e^{-\eta r} - e^{-(2\mu-\eta)r}]$, and therefore $y_0(r) = -\mu + (\mu - \eta) \coth[(\mu - \eta)r]$ where $N = \frac{\sqrt{\mu\eta(2\mu-\eta)}}{\mu-\eta}$ is the normalization factor.

Inserting this into the equation for E_0 and using a straightforward integration, one obtains for the zeroth order ground state energy

$$E_0 = \frac{\mu\eta(2\mu - \eta)}{m} \left[\frac{1}{2\mu} + \frac{\mu}{(\mu - \eta)^2} \ln \frac{(4\mu - 2\eta + \lambda)(2\eta + \lambda)}{(2\mu + \lambda)^2} \right]. \quad (2)$$

Since $E_0(\eta) = -\frac{\eta^2}{2m}$ this is a transcendental equation for the parameter η .

The first iteration of the logarithmic derivative is

given by Eq. (1). Its explicit form is given by $y_1(r) = y_0(r) + \frac{\Phi(r)}{\chi_0^2(r)}$ where [3]

$$\Phi(r) = 2\mu \left\{ \left(\frac{\eta}{\mu} - 1 \right) e^{-2\mu r} + \frac{\mu - \eta}{2\mu - \eta} e^{-2r(2\mu - \eta)} + 2Ei[-r(2\mu + \lambda)] - Ei[-r(2\eta + \lambda)] - Ei[-r(4\mu - 2\eta + \lambda)] \right\} \quad (3)$$

TABLE I: The energy values calculated by direct numerical solution of the wave equation (E_D), and in the zeroth and first iterations of QLM (E_0) and (E_1).

λ	$-E_0$	$-E_1$	$-E_D$
0.2	0.32679	0.32680851	0.32680851
0.5	0.14795	0.1481170	0.1481170
0.8	0.04445	0.0447042	0.0447043

Here $Ei(z) = -\int_{-z}^{\infty} \frac{e^{-t}}{t} dt$ is exponential integral function. Inserting $y_1(r)$ into the expression for E_1 , one can calculate the first iteration energy.

Numerical results for the binding energies are given in Table 1 while the typical modified ground state

wave function $\chi(r)$ is displayed on Fig. 1. We are using atomic system of units $m = g = 1$. The dimensionless parameter λ is expressed in units of the inverse Bohr radius while the energy E is expressed in Hartree.

Comparison of our approximate analytic expressions for binding energies and wave functions with the exact numerical solutions demonstrates their high accuracy in the wide range of physical parameters. The accuracy ranging between 10^{-4} and 10^{-8} for the energies and, correspondingly, 10^{-2} and 10^{-4} for the wave functions is reached. Similarly, the accurate analytic presentation of the solution of the Schrödinger Equation could be obtained for an arbitrary potential.

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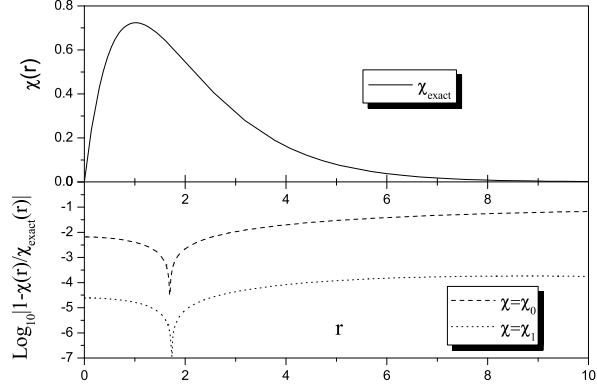


FIG. 1: Ground state wave functions for the Yukawa potential with parameter $\lambda = 0.2$. The exact modified wave function (solid line) is depicted at the upper part of the graph. Relative logarithmic deviations from the exact values for the QLM wave functions of the zeroth (dash line) and the first order (dot line) are shown in the lower part.